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Multiscale ductile fracture integrating tomographic characterization and 3-D simulation

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Abstract—Ductile fracture in alloys is a multiscale process in which primary voids formed at micron-scale particles coalesce by a zig-zag pattern of shear localization driven by finer-scale microvoiding at submicron-scale secondary particles. Employing the method of serial sectioning, unprecedented 3-D microstructural reconstructions of steel crack-tip process zones are obtained and implemented into a large-scale simulation for ductile fracture analysis. A quantitative understanding of the microvoid sheeting mechanism and mixed-mode failure controlling the zig-zag fracture surface are presented using the modeling technique utilized herein. We define and quantify metrics of fracture by analyzing the crack opening distance, process zone size, zig-zag wavelength and void growth ratios in the crack tip reconstructions. The quantitative agreement of these metrics between experiment and simulation supports a new and developing predictive structure/property theory to enable materials design.

Keywords: Ductile fracture; 3-D characterization; Multiscale simulations; Crack propagation; Serial sectioning

1. Introduction

The US Materials Genome Initiative [1] acknowledges the new opportunity of integrated computational tools grounded in fundamental databases to greatly accelerate the full materials development cycle, as already demonstrated by a new generation of "designer steels" [2] taken to full flight qualification for aircraft. While the structure–property relations enabling computational materials design [3] are well developed for material strength, the equally important property of fracture toughness, defining resistance to material fracture, has not been well represented in terms of quantitative predictive capability [4]. To address the need for such capabilities, an integrated approach of tomographic characterization and 3-D fracture simulation has been undertaken in order to bring the maturity of the structure–property relations of toughness to the same level as that of strength. Ductile fracture in steel is a process consisting of nucleation, growth and coalescence of voids and microvoids on at least two microscopic levels [5]. On the micron scale, primary voids (approximately 1–10 μm in diameter in this work) nucleate from primary inclusions that have cracked and/or debonded from the matrix. On the secondary (submicron) scale, microvoids nucleate from submicron precipitates, such as grain-refining carbides (approximately 100–200 nm in diameter in this work). The primary voids continue to grow until a critical strain level in the intervoid ligaments, where a process of microvoid softening driven by the submicron secondary microvoids acts to link the primary voids to one another by a pattern of shear localization. Rice and Johnson [6] have shown that the critical crack-tip opening displacement for crack propagation directly scales with the spacing of primary inclusions (thus, $J_{IC} \propto X_0$). This has motivated the technology of "clean steels" in which the content of inclusions governing this spacing has been substantially reduced. The linking of the primary voids by a pattern of zig-zag shear localization corresponding to microvoid sheets along paths of maximum shear strain has been well established [7,8], and the critical crack opening displacement has been shown to scale with the wavelength of this pattern [9]; however, the quantitative role of the submicron secondary particles in this pattern of shear localization has remained elusive. Our goal is to create a comprehensive model which envelops microstructure features at multiple length scales to predict fracture toughness. Based on the aforementioned characteristics of ductile fracture, toughness

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and shear instability can be determined from an examination of microstructural quantities, such as inclusion spacing, critical primary void growth ratio (final void size at fracture/inclusion size upon which the void nucleated), zig-zag wavelength of crack morphology, and crack-tip opening displacement. Many of these quantities have traditionally been experimentally measured in only two dimensions [6,7,10–15], but now with advanced tomographic capabilities developed as part of a multi-institutional effort [16], we can obtain data that is more precise, of greater statistical volume, and of 3-D character. This, in turn, supports 3-D simulation with improved quantitative validation capabilities. Previous work by Tian et al. [17] utilized the multiresolution continuum theory with purely phenomenological models used for the constitutive behavior in order to obtain an accurate depiction of a crack tip during ductile fracture. While this work did capture fracture at two length scales and included strong multiple void interaction, intervoid ligament strain analysis, a very coarse crack wavelength measurement, and an effort to relate microstructure evolution to macroscale properties, it was unable to capture the finer details of the crack both experimentally and through simulation, and lacked an explanation of the underlying mechanisms that drive the evolution of the fracture path. Thus, the present work is a notable improvement directed at determining the underlying mechanisms which govern the fracture properties and evolution of hierarchically structured alloy materials. There are a number of key features which distinguish this work as an improvement over that which was previously conducted. Experimentally, the resolution of the digital data set is seven times greater in-plane and almost two times greater section-to-section, the volume of material captured in the reconstruction is almost three times greater, and the segmentation methods are vastly improved with the utilization of color imaging and development of more advanced algorithms for automatic detection of microstructural features. This results in a more accurate depiction of the microstructure that better represents the actual process zone and provides more data for implementation and comparison with simulation (e.g. we integrated eight times more primary particles into our simulation than that used in the previous work [17]). For the simulation, we implemented the multiresolution theory and adopted two mechanics-based constitutive models for both the macro- and microzones, each of which was selected based on the mechanics known to occur during the ductile fracture process at their respective scales. A modified Gurson–Tvergaard–Needleman model is applied to the macrozone, accounting for primary void growth and shape change, and a modified Fleck–Hutchinson model is used to govern the elastic–plastic behavior in the microzone, accounting for shear localization in the microvoid region. The mechanistic nature of the models incorporated within the multiresolution theory for the current work, in combination with the vastly more extensive microstructural data available from the improved experimental techniques, yields a unified framework that is much better suited to quantify the fundamental driving forces behind the evolution of the ductile fracture process. The resulting implementation of the 3-D microstructural data into the fully mechanics-based 3-D multiscale model, combined with large-scale parallel computing capabilities, has revealed a comprehensive understanding of the fracture process including detailed micron-scale crack paths and crack branching that have not been previously captured by existing models. A summary of this implementation is given in the Supplementary Information.

2. Experimental reconstruction of a crack

Studying ductile fracture processes (void nucleation, growth and coalescence) under the conditions of engineering toughness measurement standards requires a specific mechanical test in which a plane-strain condition is achieved. This means that material must be constrained in the plane normal to the crack such that the investigated region is not subjected to shear lip deformation. We performed a modified-J_{IC} fracture toughness test on fatigue pre-cracked miniature compact-tension specimens of a titanium-modified 4330 high-strength steel; the alloy composition and processing are described elsewhere [18]. The test was halted near an estimated critical point corresponding to toughness measurement standards, to produce a specimen exhibiting the full stages of the ductile fracture process.

The crack was reconstructed in three dimensions through serial sectioning, the process of collecting a series of consecutive, closely spaced 2-D layers of images and assembling them to form a 3-D volume. Each thin layer or "slice" of material is imaged by light optical microscopy and is subsequently removed by metallographic polishing. This process of imaging and removal is repeated until over 200 sections of images are collected. To simultaneously acquire images with high resolution and with large fields of view, photomontaging is employed. Aided by an automatic stage on an optical microscope, an array of 8×8 images is collected for each slice. These overlapping images are carefully photostitched together to create one large image for each section, with an in-plane resolution of 0.133 μm per pixel and a total area of $800 \times 1000\ \mu\text{m}^2$. The depth of material removal for each section is 1.5 μm, and is tracked by fiducial marks in the form of an array of Vickers hardness indents surrounding the crack-tip region. This slice thickness was chosen as an appropriate compromise between obtaining fine microstructure detail and obtaining a large volume of data in a timely manner and with a reasonable data size. The repetitive serial sectioning process required approximately 3–4 weeks of man hours to complete. Although this is cumbersome, the more time-consuming step lies in the image processing. The photostitching (in-plane image-to-image alignment), registration (section-to-section alignment), and segmentation (identification of each microstructural feature) steps, though seemingly straightforward, required automatic and semi-automatic methods. Further details can be found in the Supplementary Information.

The crack-tip data set was reconstructed in three dimensions utilizing IDL^{TM} and Amira commercial software. IDL was used to visualize 3-D reconstructions and perform the quantitative measurements presented here, and Amira was used to create the video data included with this publication (refer to the online Supplementary Data, Movie S1). A snapshot of the fully reconstructed crack tip is represented in Fig. 1, showing the distribution of primary inclusions and the topography of the associated fracture process.

3. Simulation of ductile fracture

Taking the digital data sets from the experiments for the initial microstructure configuration, the fracture process was simulated using a multiresolution framework in which the multiscale microstructure was modeled concurrently.